Wout Bittremieux

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Employment

2022–...	**Assistant Professor** (Computer Science) University of Antwerp, Antwerp, Belgium
2019–22	**Postdoctoral Researcher** (Pharmacy and Pharmaceutical Sciences) University of California San Diego, La Jolla, CA, USA Advisor: Pieter C. Dorrestein, PhD
2017–19	**Postdoctoral Researcher** (Genome Sciences) University of Washington, Seattle, WA, USA Advisor: William Stafford Noble, PhD

Education

2013–17	**PhD in Computer Science** University of Antwerp, Antwerp, Belgium Thesis: *Computational Solutions for Quality Control of Mass Spectrometry-based Proteomics* Advisors: Kris Laukens, PhD and Bart Goethals, PhD
2016	**Visiting Researcher** Stellenbosch University, Cape Town, South Africa
2010–12	**MSc in Computer Science** Hasselt University, Diepenbeek, Belgium Thesis: *Time Series Similarity Search* Advisors: Marc Gyssens, PhD
2007–10	**BSc in Computer Science** Hasselt University, Diepenbeek, Belgium Thesis: *Extending a Web Browser With Additional Navigation Options* Advisors: Jan Van den Bussche, PhD

Awards and Honors

2025	**Junior Research Parasite**, Research Parasite Awards
2023	**Young Investigator Award**, *Metabolites*
2023	**Bioinformatics for Mass Spectrometry Award**, European Proteomics Association
2022	**Early Career Researcher Manuscript Competition Award** Human Proteome Organization
2021	**Rising Stars in Proteomics and Metabolomics: 40 Under 40** *Journal of Proteome Research*
2020	**Postdoctoral Career Development Award**, American Society for Mass Spectrometry

Updated August 20, 2025.

2015 **Best Oral Presentation Award**, Benelux Bioinformatics Conference

Peer-Reviewed Publications

[86] **Wout Bittremieux** and William Stafford Noble. "Self-Supervised Learning from Small-Molecule Mass Spectrometry Data." In: *Nature Biotechnology* (May 23, 2025), pp. 1–2. DOI: 10.1038/s41587-025-02677-x.

[85] Tim Van Den Bossche, Theodore Alexandrov, Aivett Bilbao, **Wout Bittremieux**, Federico Brigante, Matt Chambers, Joshua Charkow, Eric Deutsch, Andrew Dowsey, Yasin El Abiead, Ralf Gabriels, Helge Hecht, Steffen Heuckeroth, Joshua Klein, Michael Knierman, Lennart Martens, Robert Moritz, Laura-Isobel McCall, Steffen Neumann, Yasset Perez-Riverol, Hannes Röst, Elliott J. Price, James Shofstahl, David Tabb, Julian Uszkoreit, Juan Antonio Vizcaino, Mingxun Wang, Sander Willems, Dirk Winkelhardt, Oliver Kohlbacher, and Samuel Wein. "mzPeak: Designing a Scalable, Interoperable, and Future-Ready Mass Spectrometry Data Format." In: *Journal of Proteome Research* (In Press 2025).

[84] Charlotte Adams and **Wout Bittremieux**. "A 2025 Perspective on the Role of Machine Learning for Biomarker Discovery in Clinical Proteomics." In: *Expert Review of Proteomics* (2025). DOI: 10.1080/14789450.2025.2545828.

[83] Maarten Quireyns, Tim Boogaerts, Juan Sebastian Piedrahita Giraldo, Natan Van Wichelen, Len Feremans, Ilias Benaissati, Qëndrim Jonuzi, Bavo Verhaegen, Koenraad Van Hoorde, Hadrien Maloux, Veronik Hutse, **Wout Bittremieux**, Adrian Covaci, and Alexander L.N. Van Nuijs. "Comparing the Applicability of de Facto Population Markers for Spatiotemporal Trend Analysis in Wastewater-Based Epidemiology." In: *Journal of Hazardous Materials* 496 (Sept. 15, 2025), p. 139332. DOI: 10.1016/j.jhazmat.2025.139332.

[82] Tito Damiani, Alan K. Jarmusch, Allegra T. Aron, Daniel Petras, Vanessa V. Phelan, Haoqi Nina Zhao, **Wout Bittremieux**, Deepa D. Acharya, Mohammed M. A. Ahmed, Anelize Bauermeister, Matthew J. Bertin, Paul D. Boudreau, Ricardo M. Borges, Benjamin P. Bowen, Christopher J. Brown, Fernanda O. Chagas, Kenneth D. Clevenger, Mario S. P. Correia, William J. Crandall, Max Crüsemann, Eoin Fahy, Oliver Fiehn, Neha Garg, William H. Gerwick, Jeffrey R. Gilbert, Daniel Globisch, Paulo Wender P. Gomes, Steffen Heuckeroth, C. Andrew James, Scott A. Jarmusch, Sarvar A. Kakhkhorov, Kyo Bin Kang, Nikolas Kessler, Roland D. Kersten, Hyunwoo Kim, Riley D. Kirk, Oliver Kohlbacher, Eftychia E. Kontou, Ken Liu, Itzel Lizama-Chamu, Gordon T. Luu, Tal Luzzatto Knaan, Helena Mannochio-Russo, Michael T. Marty, Yuki Matsuzawa, Andrew C. McAvoy, Laura-Isobel McCall, Osama G. Mohamed, Omri Nahor, Heiko Neuweger, Timo H. J. Niedermeyer, Kozo Nishida, Trent R. Northen, Kirsten E. Overdahl, Johannes Rainer, Raphael Reher, Elys Rodriguez, Timo T. Sachsenberg, Laura M. Sanchez, Robin Schmid, Cole Stevens, Shankar Subramaniam, Zhenyu Tian, Ashootosh Tripathi, Hiroshi Tsugawa, Justin J. J. van der Hooft, Andrea Vicini, Axel Walter, Tilmann Weber, Quanbo Xiong, Tao Xu, Tomáš Pluskal, Pieter C. Dorrestein, and Mingxun Wang. "A Universal Language for Finding Mass Spectrometry Data Patterns." In: *Nature Methods* 22.6 (June 2025), pp. 1247–1254. DOI: 10.1038/s41592-025-02660-z.

[81] Marilyn De Graeve, **Wout Bittremieux**, Thomas Naake, Carolin Huber, Matthias Anagho-Mattanovich, Nils Hoffmann, Pierre Marchal, Victor Chrone, Philippine Louail, Helge Hecht, Michael Witting, and Johannes Rainer. "SpectriPy: Enhancing Cross-Language Mass Spectrometry Data Analysis with R and Python." In: *Journal of Open Source Software* 10.109 (May 19, 2025), p. 8070. DOI: 10.21105/joss.08070.

[80] Yasset Perez-Riverol, **Wout Bittremieux**, William S. Noble, Lennart Martens, Aivett Bilbao, Michael R. Lazear, Bjorn Grüning, Daniel S. Katz, Michael J. MacCoss, Chengxin Dai, Jimmy K. Eng, Robbin Bouwmeester, Michael R. Shortreed, Enrique Audain, Timo Sachsenberg, Jeroen Van Goey, Georg Wallmann, Bo Wen, Lukas Käll, and William E. Fondrie. "Open-Source and FAIR Research Software for Proteomics." In: *Journal of Proteome Research* 24.5 (May 2, 2025), pp. 2222–2234. DOI: 10.1021/acs.jproteome.4c01079.

[79] Xianghu Wang, Yasin El Abiead, Deepa D. Acharya, Christopher J. Brown, Ken Clevenger, Jie Hu, Ashley Kretsch, Carla Menegatti, Quanbo Xiong, **Wout Bittremieux**, and Mingxun Wang. "MS-RT: A Method for Evaluating MS/MS Clustering Performance for Metabolomics Data." In: *Journal of Proteome Research* 24.4 (Apr. 4, 2025), pp. 1778–1790. DOI: 10.1021/acs.jproteome.4c00881.

[78] Justin Cyril Sing, Joshua Charkow, Axel Walter, Mingxuan Gao, Tom David Müller, **Wout Bittremieux**, Timo Sachsenberg, and Hannes Luc Röst. "pyOpenMS-viz: Streamlining Mass Spectrometry Data Visualization with Pandas." In: *Journal of Proteome Research* 24.4 (Apr. 4, 2025), pp. 2152–2158. DOI: 10.1021/acs.jproteome.4c00873.

[77] Yasin El Abiead, Adriano Rutz, Simone Zuffa, Bashar Amer, Shipei Xing, Corinna Brungs, Robin Schmid, Mario S. P. Correia, Andres Mauricio Caraballo-Rodriguez, Amir Zarrinpar, Helena Mannochio-Russo, Michael Witting, Ipsita Mohanty, Tomáš Pluskal, **Wout Bittremieux**, Rob Knight, Andrew D. Patterson, Justin J. J. van der Hooft, Sebastian Böcker, Warwick B. Dunn, Roger G. Linington, David S. Wishart, Jean-Luc Wolfender, Oliver Fiehn, Nicola Zamboni, and Pieter C. Dorrestein. "Discovery of Metabolites Prevails amid In-Source Fragmentation." In: *Nature Metabolism* 7.3 (Mar. 2025), pp. 435–437. DOI: 10.1038/s42255-025-01239-4.

[76] Margaret R. Martin, **Wout Bittremieux**, and Soha Hassoun. "Molecular Structure Discovery for Untargeted Metabolomics Using Biotransformation Rules and Global Molecular Networking." In: *Analytical Chemistry* (2025), In Press. DOI: 10.1101/2024.02.04.578795.

[75] Stef Lauwers, Anne-Sophie Weyns, Annelies Breynaert, Tim Van Rillaer, Valerie Van Huynegem, Erik Fransen, **Wout Bittremieux**, Sarah Lebeer, Emmy Tuenter, and Nina Hermans. "Comparison of In Vitro Biotransformation of Olive Polyphenols Between Healthy Young and Elderly." In: *Metabolites* 15.1 (Jan. 7, 2025), p. 26. DOI: 10.3390/metabo15010026.

[74] Roman Bushuiev, Anton Bushuiev, Niek F. deJonge, Adamo Young, Fleming Kretschmer, Raman Samusevich, Janne Heirman, Fei Wang, Luke Zhang, Kai Dührkop, Marcus Ludwig, Nils A. Haupt, Apurva Kalia, Corinna Brungs, Robin Schmid, Russell Greiner, Bo Wang, David Wishart, Liping Liu, Juho Rousu, **Wout Bittremieux**, Hannes Rost, Tytus D. Mak, Soha Hassoun, Florian Huber, Justin J. J. van der Hooft, Michael A. Stravs, Sebastian Böcker, Josef Sivic, and Tomas Pluskal. "MassSpecGym: A Benchmark for the Discovery and Identification of Molecules." In: *Proceedings of the 38th Conference on Neural Information Processing Systems (NeurIPS 2024) Datasets and Benchmarks Track* (Dec. 9, 2024).

[73] **Wout Bittremieux**, Varun Ananth, William E. Fondrie, Carlo Melendez, Marina Pominova, Justin Sanders, Bo Wen, Melih Yilmaz, and William S. Noble. "Deep Learning Methods for De Novo Peptide Sequencing." In: *Mass Spectrometry Reviews* (Nov. 29, 2024), Early View. DOI: 10.1002/mas.21919.

[72] Joshua Klein, Henry Lam, Tytus D. Mak, **Wout Bittremieux**, Yasset Perez-Riverol, Ralf Gabriels, Jim Shofstahl, Helge Hecht, Pierre-Alain Binz, Shin Kawano, Tim Van Den Bossche, Jeremy Carver, Benjamin A. Neely, Luis Mendoza, Tomi Suomi, Tine Claeys, Thomas Payne, Douwe Schulte, Zhi Sun, Nils Hoffmann, Yunping Zhu, Steffen Neumann, Andrew R. Jones, Nuno Bandeira, Juan Antonio Vizcaíno, and Eric W. Deutsch. "The Proteomics Standards Initiative Standardized Formats for Spectral Libraries and Fragment Ion Peak Annotations: mzSpecLib and mzPAF." In: *Analytical Chemistry* 96.46 (Nov. 19, 2024), pp. 18491–18501. DOI: 10.1021/acs.analchem.4c04091.

[71] Sumukh Pinge, Weihong Xu, **Wout Bittremieux**, Niema Moshiri, Sang-Woo Jun, and Tajana Rosing. "RapidOMS: FPGA-based Open Modification Spectral Library Searching with HD Computing." In: *2024 IEEE Biomedical Circuits and Systems Conference (BioCAS)*. Xi'an, China, Oct. 2024, pp. 1–5. DOI: 10.1109/BioCAS61083.2024.10798176.

[70] Carlo Melendez, Justin Sanders, Melih Yilmaz, **Wout Bittremieux**, William E. Fondrie, Sewoong Oh, and William Stafford Noble. "Accounting for Digestion Enzyme Bias in Casanovo." In: *Journal of Proteome Research* 23.10 (Oct. 4, 2024), pp. 4761–4769. DOI: 10.1021/acs.jproteome.4c00422.

[69] Janne Heirman and **Wout Bittremieux**. "Reusability Report: Annotating Metabolite Mass Spectra with Domain-Inspired Chemical Formula Transformers." In: *Nature Machine Intelligence* 6 (Sept. 27, 2024), pp. 1296–1302. DOI: 10.1038/s42256-024-00909-4.

[68] Ceder Dens, Charlotte Adams, Kris Laukens, and **Wout Bittremieux**. "Machine Learning Strategies to Tackle Data Challenges in Mass Spectrometry-Based Proteomics." In: *Journal of the American Society for Mass Spectrometry* 35.9 (July 29, 2024), pp. 2143–2155. DOI: 10.1021/jasms.4c00180.

[67] Jaeyoung Kang, Weihong Xu, **Wout Bittremieux**, Niema Moshiri, and Tajana Rosing. "DRAM-Based Acceleration of Open Modification Search in Hyperdimensional Space." In: *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems* 43.9 (Mar. 28, 2024). DOI: 10.1109/TCAD.2024.3382842.

[66] Issar Arab, Kris Laukens, and **Wout Bittremieux**. "Semisupervised Learning to Boost hERG, Nav1.5, and Cav1.2 Cardiac Ion Channel Toxicity Prediction by Mining a Large Unlabeled Small Molecule Data Set." In: *Journal of Chemical Information and Modeling* 64.16 (Aug. 7, 2024), pp. 6410–6420. DOI: 10.1021/acs.jcim.4c01102.

[65] Chris Bielow, Nils Hoffmann, David Jimenez-Morales, Tim Van Den Bossche, Juan Antonio Vizcaíno, David L. Tabb, **Wout Bittremieux**, and Mathias Walzer. "Communicating Mass Spectrometry Quality Information in mzQC With Python, R, and Java." In: *Journal of The American Society for Mass Spectrometry* 35.8 (June 25, 2024), pp. 1875–1882. DOI: 10.1021/jasms.4c00174.

[64] Melih Yilmaz, William E. Fondrie, **Wout Bittremieux**, Carlo F. Melendez, Rowan Nelson, Varun Ananth, Sewoong Oh, and William Stafford Noble. "Sequence-to-Sequence Translation from Mass Spectra to Peptides with a Transformer Model." In: *Nature Communications* 15.1 (July 30, 2024), p. 6427. DOI: 10.1038/s41467-024-49731-x.

[63] Charlotte Adams, Wassim Gabriel, Kris Laukens, Mario Picciani, Mathias Wilhelm, **Wout Bittremieux**, and Kurt Boonen. "Fragment Ion Intensity Prediction Improves the Identification Rate of Non-Tryptic Peptides in TimsTOF." In: *Nature Communications* 15.1 (May 10, 2024), p. 3956. DOI: 10.1038/s41467-024-48322-0.

[62] Charlotte Adams, Kris Laukens, **Wout Bittremieux**, and Kurt Boonen. "Machine Learning-Based Peptide-Spectrum Match Rescoring Opens Up the Immunopeptidome." In: *PROTEOMICS* 24.8 (Apr. 2024), p. 2300336. DOI: 10.1002/pmic.202300336.

[61] Issar Arab, Kristof Egghe, Kris Laukens, Ke Chen, Khaled Barakat, and **Wout Bittremieux**. "Benchmarking of Small Molecule Feature Representations for hERG, Nav1.5, and Cav1.2 Cardiotoxicity Prediction." In: *Journal of Chemical Information and Modeling* 64.7 (Apr. 8, 2024), pp. 2515–2527. DOI: 10.1021/acs.jcim.3c01301.

[60] Ipsita Mohanty, Helena Mannochio-Russo, Joshua V. Schweer, Yasin El Abiead, **Wout Bittremieux**, Shipei Xing, Robin Schmid, Simone Zuffa, Felipe Vasquez, Valentina B. Muti, Jasmine Zemlin, Omar E. Tovar-Herrera, Sarah Moraïs, Dhimant Desai, Shantu Amin, Imhoi Koo, Christoph W. Turck, Itzhak Mizrahi, Penny M. Kris-Etherton, Kristina S. Petersen, Jennifer A. Fleming, Tao Huan, Andrew D. Patterson, Dionicio Siegel, Lee R. Hagey, Mingxun Wang, Allegra T. Aron, and Pieter C. Dorrestein. "The Underappreciated Diversity of Bile Acid Modifications." In: *Cell* 187.7 (Mar. 28, 2024), 1801–1818.e20. DOI: 10.1016/j.cell.2024.02.019.

[59] Sumukh Pinge, Weihong Xu, Jaeyoung Kang, Tianqi Zhang, Neima Moshiri, **Wout Bittremieux**, and Tajana Rosing. "SpecHD: Hyperdimensional Computing Framework for FPGA-based Mass Spectrometry Clustering." In: *Proceedings of the 2024 Design, Automation & Test in Europe Conference - DATE 2024*. Valencia, Spain, Mar. 25, 2024. DOI: 10.48550/arXiv.2311.12874.

[58] **Wout Bittremieux**, Nicole E. Avalon, Sydney P. Thomas, Sarvar A. Kakhkhorov, Alexander A. Aksenov, Paulo Wender P. Gomes, Christine M. Aceves, Andrés Mauricio Caraballo-Rodríguez, Julia M. Gauglitz, William H. Gerwick, Tao Huan, Alan K. Jarmusch, Rima F. Kaddurah-Daouk, Kyo Bin Kang, Hyun Woo Kim, Todor Kondić, Helena Mannochio-Russo, Michael J. Meehan, Alexey V. Melnik, Louis-Felix Nothias, Claire O'Donovan, Morgan Panitchpakdi, Daniel Petras, Robin Schmid, Emma L. Schymanski, Justin J. J. Van Der Hooft, Kelly C. Weldon, Heejung Yang, Shipei Xing, Jasmine Zemlin, Mingxun Wang, and Pieter C. Dorrestein. "Open Access Repository-Scale Propagated Nearest Neighbor Suspect Spectral Library For Untargeted Metabolomics." In: *Nature Communications* 14.1 (Dec. 20, 2023), p. 8488. DOI: 10.1038/s41467-023-44035-y.

[57] Ceder Dens, Kris Laukens, **Wout Bittremieux**, and Pieter Meysman. "The Pitfalls of Negative Data Bias For the T-cell Epitope Specificity Challenge." In: *Nature Machine Intelligence* 5 (Oct. 2023), pp. 1060–1062. DOI: 10.1038/s42256-023-00727-0.

[56] Ceder Dens, **Wout Bittremieux**, Fabio Affaticati, Kris Laukens, and Pieter Meysman. "Interpretable Deep Learning to Uncover the Molecular Binding Patterns Determining TCR–Epitope Interaction Predictions." In: *ImmunoInformatics* 11 (Sept. 2023), p. 100027. DOI: 10.1016/j.immuno.2023.100027.

[55] Jaeyoung Kang, Weihong Xu, **Wout Bittremieux**, Niema Moshiri, and Tajana Rosing. "Accelerating Open Modification Spectral Library Searching on Tensor Core in High-Dimensional Space." In: *Bioinformatics* 39.7 (June 27, 2023), btad404. DOI: 10.1093/bioinformatics/btad404.

[54] Weihong Xu, Jaeyoung Kang, **Wout Bittremieux**, Niema Moshiri, and Tajana Rosing. "HyperSpec: Ultrafast Mass Spectra Clustering in Hyperdimensional Space." In: *Journal of Proteome Research* 22.6 (June 2, 2023), pp. 1639–1648. DOI: 10.1021/acs.jproteome.2c00612.

[53] **Wout Bittremieux**, Lev Levitsky, Matteo Pilz, Timo Sachsenberg, Florian Huber, Mingxun Wang, and Pieter C. Dorrestein. "Unified and Standardized Mass Spectrometry Data Processing in Python Using spectrum_utils." In: *Journal of Proteome Research* 22.2 (Feb. 3, 2023), pp. 625–631. DOI: 10.1021/acs.jproteome.2c00632.

[52] Issar Arab, William E. Fondrie, Kris Laukens, and **Wout Bittremieux**. "Semisupervised Machine Learning for Sensitive Open Modification Spectral Library Searching." In: *Journal of Proteome Research* 22.2 (Feb. 3, 2023), pp. 585–593. DOI: 10.1021/acs.jproteome.2c00616.

[51] Eric W. Deutsch, Juan Antonio Vizcaíno, Andrew R. Jones, Pierre-Alain Binz, Henry Lam, Joshua Klein, **Wout Bittremieux**, Yasset Perez-Riverol, David L. Tabb, Mathias Walzer, Sylvie Ricard-Blum, Henning Hermjakob, Steffen Neumann, Tytus D. Mak, Shin Kawano, Luis Mendoza, Tim Van Den Bossche, Ralf Gabriels, Nuno Bandeira, Jeremy Carver, Benjamin Pullman, Zhi Sun, Nils Hoffmann, Jim Shofstahl, Yunping Zhu, Luana Licata, Federica Quaglia, Silvio C. E. Tosatto, and Sandra E. Orchard. "Proteomics Standards Initiative at Twenty Years: Current Activities and Future Work." In: *Journal of Proteome Research* 22.2 (Feb. 3, 2023), pp. 287–301. DOI: 10.1021/acs.jproteome.2c00637.

[50] Julia M. Gauglitz, Kiana A. West, **Wout Bittremieux**, Candace L. Williams, Kelly C. Weldon, Morgan Panitchpakdi, Francesca Di Ottavio, Christine M. Aceves, Elizabeth Brown, Nicole C. Sikora, Alan K. Jarmusch, Cameron Martino, Anupriya Tripathi, Michael J. Meehan, Kathleen Dorrestein, Justin P. Shaffer, Roxana Coras, Fernando Vargas, Lindsay DeRight Goldasich, Tara Schwartz, MacKenzie Bryant, Gregory Humphrey, Abigail J. Johnson, Katharina Spengler, Pedro Belda-Ferre, Edgar Diaz, Daniel McDonald, Qiyun Zhu, Emmanuel O. Elijah, Mingxun Wang, Clarisse Marotz, Kate E. Sprecher, Daniela Vargas-Robles, Dana Withrow, Gail Ackermann, Lourdes Herrera, Barry J. Bradford, Lucas Maciel Mauriz Marques, Juliano Geraldo Amaral, Rodrigo Moreira Silva, Flavio Protasio Veras, Thiago Mattar Cunha, Rene Donizeti Ribeiro Oliveira, Paulo Louzada-Junior, Robert H. Mills, Paulina K. Piotrowski, Stephanie L. Servetas, Sandra M. Da Silva, Christina M. Jones, Nancy J. Lin, Katrice A. Lippa, Scott A. Jackson, Rima Kaddurah Daouk, Douglas Galasko, Parambir S. Dulai, Tatyana I. Kalashnikova, Curt Wittenberg, Robert Terkeltaub, Megan M. Doty, Jae H. Kim, Kyung E. Rhee, Julia Beauchamp-Walters, Kenneth P. Wright, Maria Gloria Dominguez-Bello, Mark Manary, Michelli F. Oliveira, Brigid S. Boland, Norberto Peporine Lopes, Monica Guma, Austin D. Swafford, Rachel J. Dutton, Rob Knight, and Pieter C. Dorrestein. "Enhancing Untargeted Metabolomics Using Metadata-Based Source Annotation." In: *Nature Biotechnology* 40 (Dec. 2022), pp. 1774–1779. DOI: 10.1038/s41587-022-01368-1.

[49] Justin P. Shaffer, Louis-Félix Nothias, Luke R. Thompson, Jon G. Sanders, Rodolfo A. Salido, Sneha P. Couvillion, Asker D. Brejnrod, Franck Lejzerowicz, Niina Haiminen, Shi Huang, Holly L. Lutz, Qiyun Zhu, Cameron Martino, James T. Morton, Smruthi Karthikeyan, Mélissa Nothias-Esposito, Kai Dührkop, Sebastian Böcker, Hyun Woo Kim, Alexander A. Aksenov, **Wout Bittremieux**, Jeremiah J. Minich, Clarisse Marotz, MacKenzie M. Bryant, Karenina Sanders, Tara Schwartz, Greg Humphrey, Yoshiki Vásquez-Baeza, Anupriya Tripathi, Laxmi Parida, Anna Paola Carrieri, Kristen L. Beck, Promi Das, Antonio González, Daniel McDonald, Joshua Ladau, Søren M. Karst, Mads Albertsen, Gail Ackermann, Jeff DeReus, Torsten Thomas, Daniel Petras, Ashley Shade, James Stegen, Se Jin Song, Thomas O. Metz, Austin D. Swafford, Pieter C. Dorrestein, Janet K. Jansson, Jack A. Gilbert, Rob Knight, the Earth Microbiome Project 500 (EMP500) Consortium, Lars T. Angenant, Alison M. Berry, Leonora S. Bittleston, Jennifer L. Bowen, Max Chavarría, Don A. Cowan, Dan Distel, Peter R. Girguis, Jaime Huerta-Cepas, Paul R. Jensen, Lingjing Jiang, Gary M. King, Anton Lavrinienko, Aurora MacRae-Crerar, Thulani P. Makhalanyane, Tapio Mappes, Ezequiel M. Marzinelli, Gregory Mayer, Katherine D. McMahon, Jessica L. Metcalf, Sou Miyake, Timothy A. Mousseau, Catalina Murillo-Cruz, David Myrold, Brian Palenik, Adrián A. Pinto-Tomás, Dorota L. Porazinska, Jean-Baptiste Ramond, Forest Rowher, Taniya RoyChowdhury, Stuart A. Sandin, Steven K. Schmidt, Henning Seedorf, Ashley Shade, J. Reuben Shipway, Jennifer E. Smith, James Stegen, Frank J. Stewart, Karen Tait, Torsten Thomas, Yael Tucker, Jana M. U'Ren, Phillip C. Watts, Nicole S. Webster, Jesse R. Zaneveld, and Shan Zhang. "Standardized Multi-Omics of Earth's Microbiomes Reveals Mi-

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[45] **Wout Bittremieux**, Robin Schmid, Florian Huber, Justin J.J. van der Hooft, Mingxun Wang, and Pieter C. Dorrestein. "Comparison of Cosine, Modified Cosine, and Neutral Loss Based Spectrum Alignment For Discovery of Structurally Related Molecules." In: *Journal of The American Society for Mass Spectrometry* 33.9 (Sept. 7, 2022), pp. 1733–1744. DOI: 10.1021/jasms.2c00153.

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[15] Ralf Gabriëls, **Wout Bittremieux**, and Robbin Bouwmeester. "Machine Learning for Proteomics: Challenges, Opportunities, and ProteomicsML." 72nd ASMS Conference on Mass Spectrometry and Allied Topics (ASMS 2024). June 5, 2024. DOI: 10.5281/zenodo.13710549.

[14] Melih Yilmaz, **Wout Bittremieux**, and Konstantinos Kalogeropoulos. "De Novo Peptide Sequencing: Breakthroughs and Challenges." 72nd ASMS Conference on Mass Spectrometry and Allied Topics (ASMS 2024). Sept. 6, 2024. DOI: 10.5281/zenodo.13710568.

[13] **Wout Bittremieux**. "Improved Immunopeptidome Analysis Using timsTOF Fragment Ion Intensity Prediction." OMICS Research Day. May 15, 2024. DOI: 10.5281/zenodo.13710599.

[12] **Wout Bittremieux**. "Molecules of Mystery: A Journey of Computational Mass Spectrometry and Artificial Intelligence." Faculty of Science Research Day. Feb. 8, 2024. DOI: 10.5281/zenodo.10638649.

[11] **Wout Bittremieux**. "Bioinformatics to Explore the Molecular Universe." In: *EuPA ECR Day* (Oct. 5, 2023). DOI: 10.5281/zenodo.8411347.

[10] **Wout Bittremieux**. "Sequence-to-Sequence Translation from Mass Spectra to Peptides with a Transformer Model." In: *Proteomics ONLINE Webinar* (Sept. 18, 2023). DOI: 10.5281/zenodo.8395305.

[9] **Wout Bittremieux**. "Machine Learning Applications for Immunopeptidomics Analysis." In: *Bioinformatics Hub, HUPO 2023 World Congress* Busan, South Korea (Sept. 18, 2023). DOI: 10.5281/zenodo.8353779.

[8] **Wout Bittremieux**. "Deep Learning to Uncover the Immunopeptidome." In: *43rd BMSS Annual Meeting* Manchester, United Kingdom (Sept. 14, 2023). DOI: 10.5281/zenodo.8346713.

[7] **Wout Bittremieux**. "Leveraging Public Mass Spectrometry for Molecular Discovery from Millions of Mass Spectra." In: *Biomina Lunch Talks* Antwerp, Belgium (June 30, 2023). DOI: 10.5281/zenodo.8171855.

[6] **Wout Bittremieux**. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *HUPO Annual Conference* Cancun, Mexico (Dec. 7, 2022).

[5] **Wout Bittremieux**. "Introduction to Machine Learning." In: *Imaging Mass Spectrometry Workshop, ASMS Annual Conference* Minneapolis, MN, USA (June 7, 2022).

[4] **Wout Bittremieux**. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *Best of US HUPO 2022* (May 3, 2022). DOI: 10.5281/ZENODO.6515099.

[3] **Wout Bittremieux**. "Leveraging Public Untargeted Metabolomics Data to Propagate Structurally Related Molecule Annotations to Millions of MS/MS Spectra." In: *Applied Bioinformatics in Life Sciences* Leuven, Belgium (Mar. 11, 2022). DOI: 10.5281/ZENODO.6346949.

[2] **Wout Bittremieux**. "Shedding Light on Complex Mass Spectrometry Proteomics Processes through Advanced Data Mining." In: *Faculty of Science Research Day* Antwerp, Belgium (Jan. 13, 2017). DOI: 10.5281/zenodo.242392.

[1] **Wout Bittremieux**. "iMonDB: Mass Spectrometry Instrument Monitoring for Quality Control." In: *Methods and Tools for Intra- and Inter-experiment LC MS Performance Tracking Workshop, ASMS Annual Conference* St. Louis, MO, USA (June 1, 2015).

Oral Presentations

[14] **Wout Bittremieux**. "Sequence-to-Sequence Translation from Mass Spectra to Peptides with a Transformer Model." EuBIC-MS Seminar on Computational Mass Spectrometry. Sept. 26, 2024. DOI: 10.5281/zenodo.13880095.

[13] Charlotte Adams, Wassim Gabriel, Kris Laukens, Mathias Wilhelm, Kurt Boonen, and **Wout Bittremieux**. "Improved Immunopeptidome Analysis Using timsTOF Fragment Ion Intensity Prediction." BSPR-EuPA 2023. July 19, 2023. DOI: 10.5281/zenodo.8163554.

[12] **Wout Bittremieux**. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *US HUPO 2022* Charleston, SC, USA (Mar. 1, 2022). DOI: 10.5281/ZENODO.6320843.

[11] **Wout Bittremieux**, Julia Gauglitz, Alexander Aksenov, Alan K Jarmusch, Louis-Felix Nothias, Daniel Petras, Mingxun Wang, and Pieter C Dorrestein. "Repository-Scale Propagated Spectral Library of Suspects." In: *SoCal Science @Home Lollapalooza* (Dec. 1, 2020). DOI: 10.5281/zenodo.4300710.

[10] **Wout Bittremieux**, Damon H May, Jeffrey Bilmes, and William Stafford Noble. "Deep Neural Network Embedding for Efficient Repository-Scale Analysis of Hundreds of Millions of Mass Spectra." In: *ASMS 2020 Reboot* (June 8, 2020). DOI: 10.5281/zenodo.3831052.

[9] **Wout Bittremieux**. "Identifying Millions of Protein Modifications Using GPU-powered Approximate Nearest Neighbor Searching." In: *GPU Technology Conference* (Mar. 26, 2020). DOI: 10.5281/zenodo.3831055.

[8] **Wout Bittremieux**, Pieter Meysman, William Stafford Noble, and Kris Laukens. "Fast Open Modification Spectral Library Searching through Approximate Nearest Neighbor Indexing." In: *Cascadia Proteomics Symposium* Seattle, WA, USA (July 23, 2018). DOI: 10.5281/zenodo.1319035.

[7] **Wout Bittremieux**. "Git: How Version Control Can Power Your Research." In: *Biomina Lunch Talks* Antwerp, Belgium (June 24, 2016). DOI: 10.5281/zenodo.56352.

[6] **Wout Bittremieux**, Dirk Valkenborg, and Kris Laukens. "Optimized Open Modification Spectral Library Searching Using Approximate Nearest Neighbor Techniques." In: *ASMS Annual Conference* San Antonio, TX, USA (June 9, 2016). DOI: 10.5281/zenodo.55999.

[5] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Bart Goethals, Dirk Valkenborg, and Kris Laukens. "Approaches for Mass Spectrometry Quality Control." In: *Biomina Research Day* Antwerp, Belgium (Dec. 9, 2015). DOI: 10.5281/zenodo.56004.

[4] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Bart Goethals, Dirk Valkenborg, and Kris Laukens. "Analysis of Mass Spectrometry Quality Control Metrics." In: *Benelux Bioinformatics Conference* Antwerp, Belgium (Dec. 7, 2015). DOI: 10.5281/zenodo.56001.

[3] **Wout Bittremieux** and Kris Laukens. "Precursor-Free and Fast Spectral Library Search Using Approximate Nearest Neighbor Techniques." In: *Benelux Bioinformatics Conference Student Council Symposium* Antwerp, Belgium (Dec. 6, 2015). DOI: 10.5281/zenodo.56002.

[2] **Wout Bittremieux**, Emmanuel Müller, Dirk Valkenborg, Lennart Martens, Bart Goethals, and Kris Laukens. "Pattern Mining of Mass Spectrometry Quality Control Data." In: *Benelux Bioinformatics Conference* Luxembourg, Luxembourg (Dec. 9, 2014). DOI: 10.5281/zenodo.56000.

[1] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, and Kris Laukens. "Collecting and Mining Mass Spectrometry Quality Control Data." In: *Biomina Research Day* Antwerp, Belgium (Feb. 20, 2014). DOI: 10.5281/zenodo.56003.

Poster Presentations

[18] Marina Pominova, Charlotte Adams, Ceder Dens, and **Wout Bittremieux**. "A Living Proteomics Benchmark for Comprehensive Evaluation of Deep Learning-Based de Novo Peptide Sequencing Tools." June 3, 2025. DOI: 10.5281/zenodo.15628888.

[17] Janne Heirman and **Wout Bittremieux**. "Enhanced Spectrum Clustering for Molecular Networking." June 3, 2024. DOI: 10.5281/zenodo.13710484.

[16] **Wout Bittremieux**, Lev Levitsky, Matteo Pilz, Timo Sachsenberg, Florian Huber, Mingxun Wang, and Pieter C. Dorrestein. "Unified and Standardized Mass Spectrometry Data Processing in Python Using Spectrum_utils." June 5, 2023. DOI: 10.5281/zenodo.7987183.

[15] Charlotte Adams, Issar Arab, William E. Fondrie, Kurt Boonen, Kris Laukens, and **Wout Bittremieux**. "Semi-Supervised Rescoring For Open Modification Searching Reveals Protein Modifications During SARS-CoV-2 Infection." In: *HUPO Annual Conference* Cancun. Mexico (Dec. 6, 2022).

[14] **Wout Bittremieux**. "Comparison of Spectrum Similarity Measures for Discovery of Structurally Related Molecules." In: *ASMS Annual Conference* Minneapolis, MN, USA (June 8, 2022). DOI: 10.5281/ZENODO.6609002.

[13] **Wout Bittremieux**. "Leveraging Public Untargeted Metabolomics Data to Propagate Annotations to Millions of MS/MS Spectra." In: *US HUPO 2022* Charleston, SC, USA (Mar. 1, 2022). DOI: 10.5281/ZENODO.6303580.

[12] **Wout Bittremieux**, Sydney P Thomas, Mingxun Wang, and Pieter C Dorrestein. "Repository Scale Propagated Spectral Library of Suspects for Untargeted Metabolomics." In: *ASMS Annual Conference* Philadelphia, PA, USA (Nov. 2, 2021). DOI: 10.5281/ZENODO.5609253.

[11] **Wout Bittremieux**, Damon H May, Jeffrey Bilmes, and William Stafford Noble. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *Machine Learning in Computational Biology* Vancouver, BC, Canada (Dec. 14, 2019). DOI: 10.5281/zenodo.3576516.

[10] **Wout Bittremieux**, Kris Laukens, and William Stafford Noble. "ANN-SoLo: Extremely Fast and Accurate Open Modification Spectral Library Searching." In: *ASMS Annual Conference* Atlanta, GA, USA (June 3, 2019). DOI: 10.5281/zenodo.3242687.

[9] **Wout Bittremieux**, Pieter Meysman, William Stafford Noble, and Kris Laukens. "Fast Open Modification Spectral Library Searching through Approximate Nearest Neighbor Indexing." In: *Department of Genome Sciences Retreat* Leavenworth, WA, USA (Sept. 17, 2018). DOI: 10.5281/zenodo.1418397.

[8] **Wout Bittremieux**, Dirk Valkenborg, and Kris Laukens. "Towards the Smart Lab: A Comprehensive Approach to Mass Spectrometry Quality Control." In: *ASMS Annual Conference* Indianapolis, IN, USA (June 8, 2017). DOI: 10.5281/zenodo.584052.

[7] **Wout Bittremieux** and Kris Laukens. "Mass Spectrometry Proteomics: Ready for the Deep Learning (r)Evolution?" In: *ASMS Annual Conference* Indianapolis, IN, USA (June 8, 2017). DOI: 10.5281/zenodo.584067.

[6] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Dirk Valkenborg, and Kris Laukens. "Automatic Quality Assessment of Mass Spectrometry Experiments by Multivariate Quality Control Metrics." In: *ASMS Annual Conference* San Antonio, TX, USA (June 9, 2016). DOI: 10.5281/zenodo.55998.

[5] **Wout Bittremieux**, Hanny Willems, Lennart Martens, Dirk Valkenborg, and Kris Laukens. "Mass Spectrometry Quality Control: Instrument Monitoring and Pattern Mining Insights." In: *ASMS Annual Conference* St. Louis, MO, USA (June 2, 2015). DOI: 10.5281/zenodo.55992.

[4] **Wout Bittremieux**, Hanny Willems, Lennart Martens, Bart Goethals, Dirk Valkenborg, and Kris Laukens. "A Comprehensive Approach to Mass Spectrometry Quality Control." In: *Two-day Symposium of the Belgian Proteomics Association* Brussels, Belgium (Dec. 18, 2014). DOI: 10.5281/zenodo.55990.

[3] **Wout Bittremieux**, Dirk Valkenborg, Aida Mrzic, Hanny Willems, Bart Goethals, and Kris Laukens. "Pattern Mining of Mass Spectrometry Quality Control Data." In: *European Conference on Computational Biology* Strasbourg, France (Sept. 7, 2014). DOI: 10.5281/zenodo.55989.

[2] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, Bart Goethals, and Kris Laukens. "Mining Mass Spectrometry Quality Control Data." In: *ASMS Annual Conference* Baltimore, MD, USA (June 16, 2014). DOI: 10.5281/zenodo.55988.

[1] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, and Kris Laukens. "jqcML: An Open-Source Java API for Mass Spectrometry Quality Control Data in the qcML Format." In: *Benelux Bioinformatics Conference* Brussels, Belgium (Dec. 9, 2013). DOI: 10.5281/zenodo.55986.

Supervision of Researchers

Postdoctoral Supervision

Gaetan De Waele, Computer Science, University of Antwerp 2025/10 – ...
Prior Degree: PhD in Bioscience Engineering, Ghent University, Belgium, 2025
Project: Deep Learning For Discovery of Molecules Not Identifiable Through Library Searching

Charlotte Adams, Computer Science, University of Antwerp 2024/12 – ...
Prior Degree: PhD in Science, University of Antwerp, Belgium, 2024
Project: Privacy in Proteomics: Safeguarding Personally Identifiable Information in Clinical Omics Data

Ceder Dens, Computer Science, University of Antwerp 2024/10 – ...
Prior Degree: PhD in Computer Science, University of Antwerp, Belgium, 2024
Project: *De Novo* Mass Spectrometry Peptide Sequencing With a Transformer Large Language Model

Juan Sebastian Piedrahita Giraldo, Computer Science, University of Antwerp 2023/10 – ...
Prior Degree: PhD in Computer Science, KU Leuven, Belgium, 2021
Project: Deep Learning for Comprehensive Small Molecule Discovery From Untargeted Mass Spectrometry Data

PhD Supervision

Samer Makni, Computer Science, University of Antwerp 2025/09 – …
Prior Degree: MSc in Computer Science Engineering, Óbuda University, Hungary, 2025
Project: Artificial Intelligence to Uncover Patterns in Mass Spectrometry Data Across Repositories

Fatemeh Mirzadeh Sarcheshmeh, Computer Science, University of Antwerp 2025/09 – …
Prior Degree: MSc in Mechatronics Engineering, University of Tehran, Iran, 2024
Project: AI-Driven Metadata Annotation and Quality Control for Reproducible Mass Spectrometry-Based Omics Research

Moira Breëns, Computer Science, University of Antwerp 2025/02 – …
Prior Degree: MSc in Biochemistry and Biotechnology, University of Antwerp, Belgium, 2024
Project: Bioinformatics Solutions For the Comprehensive Study of the Human Immunopeptidome

Alejandro Mendoza Cantu, Science, University of Antwerp 2024/05 – …
Prior Degree: MSc in Agricultural & Food Data Management, UniLaSalle, France, 2023
Project: Reference Data-Driven Metabolomics to Study the Molecular Composition of South African Foods

Marina Pominova, Computer Science, University of Antwerp 2024/02 – …
Prior Degree: MSc in Computer Science, Skolkovo Institute of Science and Technology, Russia, 2020
Project: Computational Mass Spectrometry and Artificial Intelligence to Unravel the Immunopeptidome

Madina Bekbergenova, Computer Science, University of Antwerp 2023/12 – …
Prior Degree: MSc in Mathematics, University of Côte d'Azur, France, 2023
Project: Deep Reinforcement Learning for Mass Spectrometry Data Acquisition in Metabolomics

Janne Heirman, Computer Science, University of Antwerp 2023/09 – …
Prior Degree: MSc in Engineering: Computer Science, KU Leuven, Belgium, 2022
Project: Bioinformatics and Machine Learning For Large-Scale Metabolomics Data Analysis

Issar Arab, Computer Science, University of Antwerp 2022/02 – …
Prior Degree: MSc in Computer Science, Technical University Munich, Germany, 2020
Project: Open Modification Search Methods for Tandem Mass Spectrometry

Charlotte Adams, Science, University of Antwerp 2020/12 – 2024/11
Prior Degree: MSc in Biochemistry and Biotechnology, University of Antwerp, Belgium, 2020
Project: Bioinformatics Approaches to Unravel Hidden Knowledge From Mass Spectrometry-Based Proteomics Data

Ceder Dens, Computer Science, University of Antwerp 2020/12 – 2024/09
Prior Degree: MSc in Computer Science, University of Antwerp, Belgium, 2020
Project: Artificial Intelligence to Decode the Peptide Sequences Driving the Immune Response

MSc Supervision

Saartje Herman, Computer Science, University of Antwerp 2024/09 – …
Project: Contrastive Learning With Spectrum Transformers For Large-Scale Proteomics Data Analysis

Lotte Thys, Computer Science, University of Antwerp 2024/09 – 2025/09
Project: Detecting Foreign Peptides in Human Proteomics Data Using *De Novo* Peptide Sequencing

Dries De Ryck, Computer Science, University of Antwerp 2024/09 – 2025/06
Project: Double Machine Learning to Uncover Causal Microbe–Metabolite Relationships

Michel Dierckx, Computer Science, University of Antwerp 2024/09 – 2025/06
Project: Scalable Mass-Spectrometry-Based Molecular Phylogeny with TreeMS2

Viktor Hura, Computer Science, University of Antwerp 2024/09 – 2025/06
Project: Machine Learning-Based Prediction of VCD Spectra For Molecular Mirror Images

Wannes Lamberts, Computer Science, University of Antwerp 2024/09 – 2025/06
Project: Context-Aware Retention Time Prediction For Enhanced Proteomics Analysis

Cédric Leclercq, Computer Science, University of Antwerp 2024/09 – 2025/06
Project: Uncovering Maternal Drug Exposure Through Positive-Unlabeled Learning of Breast Milk Metabolomics

Dzhem Myumyun, Computer Science, University of Antwerp 2024/09 – 2025/06
Project: AI-Driven ECG Pattern Recognition For Inherited Cardiac Arrhythmia and Cardiomyopathy

Mathieu Maessen, Biomedical Sciences, University of Antwerp 2024/01 – 2024/09
Project: Exploring the Evolutionary Presence of Post-Translational Modifications Through Public Mass Spectrometry-Based Proteomics Data Reanalysis

Teaching

Training

2022	The Carpentries Instructor Training

Experience

2024–...	Biomedical Artificial Intelligence: Instructor, University of Antwerp – Master of Computer Science
2024–...	Machine Learning: Instructor, University of Antwerp – Master Biochemistry and Biotechnology
2024–...	Introduction to Computational Biology: Instructor, University of Antwerp – Bachelor of Computer Science
2022–...	Fundamentals of Machine Learning for Mass Spectrometry Data Analysis: Instructor, American Society for Mass Spectrometry – Annual Conference Short Course
2021	System-Wide Mass Spectrometry: Guest Lecturer, University of California San Diego – Cellular & Molecular Medicine
2017	Introduction to Computational Biology: Teaching Assistant, University of Antwerp – Bachelor of Computer Science
2016	Project Work: Teaching Assistant, University of Antwerp – Bachelor of Mathematics
2014–15	Data Mining: Teaching Assistant, University of Antwerp – Master of Biochemistry and Biotechnology
2015	Data Mining: Guest Lecturer, University of Antwerp – Master of Computer Science

Funding Acquired

Current Support

BOF 23-AWP-COE-11 (Covaci) 2026/01/01 – 2031/12/31
University of Antwerp – University Research Fund €720,000
Exposomics: A Holistic Approach to Assess Environmental Exposures and Their Impact on Endocrine and Metabolic Disorders
Role: Co-PI

VLAIO HBC.2025.0264 (Bittremieux) 2025/11/01 – 2027/10/31
VLAIO (Agentschap Innoveren & Ondernemen) €340,500
De Novo Mass Spectrometry Peptide Sequencing With a Transformer Large Language Model
Role: PI

FWO 12A0226N (Bittremieux) 2025/11/01 – 2028/10/31
Research Foundation – Flanders €312,440
Privacy in Proteomics: Safeguarding Personally Identifiable Information in Clinical Omics Data
Role: PI

BOF 54966-International Joint PhD (Bittremieux) 2025/10/01 – 2026/03/31
University of Antwerp – University Research Fund €28,000
Deep Reinforcement Learning for Mass Spectrometry Data Acquisition in Metabolomics
Role: PI

IOF POC CREATE 54225 (Bittremieux) 2025/09/01 – 2026/08/31
University of Antwerp – Industrial Research Fund €125,000
Accurate and Scalable AI-Driven De Novo Sequencing For Immunopeptide Discovery
Role: PI

VLIRUOS SI2025SEL158 (Bittremieux) 2025/09/01 – 2027/08/31
VLIR (Flemish Interuniversities Council) €70,000
Studying the Molecular Composition of Endemic, Heirloom, and Unconventional Foods in the Philippines
Role: PI

BOF 53845-Research Infrastructure (Ellender) 2025/06/01 – 2027/05/31
University of Antwerp – University Research Fund €150,000
Novel 3D Multi-Electrode Technology to Record From Complex Electrically Excitable Tissues and Organoids
Role: Co-PI

FWO G0AHY25N (Bittremieux) 2025/01/01 – 2028/12/31
Research Foundation – Flanders €656,500
Artificial Intelligence to Uncover Patterns in Mass Spectrometry Data Across Repositories
Role: PI

FWO G087625N (Bittremieux) 2025/01/01 – 2028/12/31
Research Foundation – Flanders €617,000
Bioinformatics Solutions For the Comprehensive Study of the Human Immunopeptidome
Role: PI

IOF POC CREATE 53170 (Bittremieux) 2025/01/01 – 2025/12/31
University of Antwerp – Industrial Research Fund €125,000
The Live Mouse Tracker (LMT) as a Versatile Drug Screening Platform For Rare Neurological Diseases
Role: PI

FWO 12A4025N (Bittremieux) 2024/10/01 – 2027/09/30
Research Foundation – Flanders €332,940
Deep Learning For Comprehensive Small Molecule Discovery From Untargeted Mass Spectrometry Data
Role: PI

FWO G0AGQ24N (Bittremieux) 2024/01/01 – 2026/12/31
Research Foundation – Flanders €314,450
Reference Data-Driven Metabolomics to Study the Molecular Composition of South African Foods
Role: PI

FWO W000924N (Bittremieux) 2024/01/01 – 2028/12/31
Research Foundation – Flanders €60,000
Bioinformatics Network For Proteomics and Mass Spectrometry
Role: PI

SPECTRUM (Nothias) 2023/12/01 – 2026/11/30
University of the Côte d'Azur
Deep Reinforcement Learning for Mass Spectrometry Data Acquisition in Metabolomics
Role: Co-PI

BOF 49083-DOCPRO2023 (Bittremieux) 2023/10/01 – 2027/09/30
University of Antwerp – University Research Fund €245,000
Computational Mass Spectrometry and Artificial Intelligence to Unravel the Immunopeptidome
Role: PI

BOF 49298-DOCPRO2022 (Bittremieux) 2022/12/01 – 2026/11/30
University of Antwerp – University Research Fund €225,000
Bioinformatics and Machine Learning For Large-Scale Metabolomics Data Analysis
Role: PI

IOF Technology Consortia 43019 (Laukens) 2021/01/01 – 2026/12/31
University of Antwerp – Industrial Research Fund €440,000
Precision Medicine Technologies (PreMeT)
Role: co-PI

Previous Support

IOF POC CREATE 51155 (Bittremieux) 2024/05/01 – 2025/05/30
University of Antwerp – Industrial Research Fund €125,000
De Novo Mass Spectrometry Peptide Sequencing With a Transformer Large Language Model
Role: PI

POC-PP 49336 (Laukens) 2023/05/01 – 2024/12/31
Plan Flemish Resilience – Infectious Diseases & Environmental Health €161,423
Enabling Mobile and Data-Driven Pathogen Monitoring Through a Paired Nanopore Squiggle–Genome Sequence Database
Role: Co-PI

NIH 1R03OD034493-01 (Dorrestein) 2022/09/01 – 2023/08/31
National Institutes of Health $302,764
Cross Repository Metabolomics Data and Workflow Integration
Role: Co-Investigator

BOF 40004-DOCPRO2019 (Laukens) 2019/10/01 – 2023/09/30
University of Antwerp – University Research Fund €205,000
Transferable Deep Learning for Sequence Based Prediction of Molecular Interactions
Role: Co-PI

BAEF 2017-FELLOW-E060 (Bittremieux) 2018/07/01 – 2019/06/30
Belgian American Educational Foundation $45,000
Prediction of Mass Spectrometry Spectral Libraries
Role: Postdoctoral Fellow

FWO 12W0418N (Bittremieux) 2017/10/01 – 2020/07/31
Research Foundation – Flanders €265,300
Intelligent Quality Control for Mass Spectrometry-based Proteomics
Role: Postdoctoral Fellow

Professional Activities

Referee

Journals. Analytical Chemistry; Artificial Intelligence in Medicine; Bioinformatics; Bioinformatics Advances; BMC Bioinformatics; Cell; Cell Metabolism; Communications Biology; Communications Chemistry; Genome Biology; Genomics, Proteomics & Bioinformatics; IEEE/ACM Transactions on Computational Biology and Bioinformatics; Journal of the American Society for Mass Spectrometry; Journal of Computational Biology; Journal of Open Source Software; Journal of Proteome Research; Mass Spectrometry Reviews; Metabolites; Nature Biotechnology; Nature Communications; Nature Machine Intelligence; PLOS Computational Biology; PLOS ONE; PROTEOMICS; Scientific Reports

Conferences. European Conference on Computational Biology (ECCB), Intelligent Systems for Molecular Biology (ISMB), Machine Learning in Computational Biology (MLCB), NIPS Workshop on Machine Learning in Computational Biology, Research in Computational Molecular Biology (RECOMB), Workshop on Data Mining in Bioinformatics (BIOKDD)

Funding. Boehringer Ingelheim Stiftung, German Research Foundation (DFG), Natural Sciences and Engineering Research Council of Canada (NSERC)

Editor

Guest editor for PLOS Computational Biology and PROTEOMICS.

Scientific Meetings Organized

2026	Benelux Metabolomics Days (Antwerp, Belgium): Main Organizer
2025	Intelligent Systems for Molecular Biology / European Conference on Computational Biology (Liverpool, UK) – Computational Mass Spectrometry Track: Chair
2025	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Neustift, Italy): Organizing Committee Member
2024	National Synthesis Center for Emergence in the Molecular and Cellular Sciences Summit Meeting (Chicago, IL, USA): Thematic Chair
2024	European Bioinformatics Community for Mass Spectrometry – ProteoBench Workshop (Ghent, Belgium): Main Organizer
2024	Intelligent Systems for Molecular Biology (Montreal, QC, Canada) – Computational Mass Spectrometry Track: Chair
2023	Intelligent Systems for Molecular Biology / European Conference on Computational Biology (Lyon, France) – Computational Mass Spectrometry Track: Chair
2022	Intelligent Systems for Molecular Biology (Madison, WI, USA) – Computational Mass Spectrometry Track: Chair
2022	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Oeiras, Portugal): Organizing Committee Member
2022	US HUPO Annual Conference (Charleston, SC, USA) – Computational Proteomics: From Machine Learning to Human Insight Track: Chair
2021	American Society for Mass Spectrometry Annual Conference (Philadelphia, PA, USA) – Quality Control Workshop: Chair
2021	Intelligent Systems for Molecular Biology / European Conference on Computational Biology (online) – Computational Mass Spectrometry Track: Chair
2020	Intelligent Systems for Molecular Biology Conference (online) – Computational Mass Spectrometry Track: Co-chair
2020	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Nyborg, Denmark): Organizing Committee Member

2019	Machine Learning in Computational Biology (Vancouver, BC, Canada): Program Committee Member
2019	European Bioinformatics Community for Mass Spectrometry Winter School (Zakopane, Poland): Organizing Committee Member
2018	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Ghent, Belgium): Main Organizer
2015	Benelux Bioinformatics Community (Antwerp, Belgium): Organizing Committee Member
2014	Belgian Proteomics Association Symposium (Brussels, Belgium): Local Organizing Committee Member

Professional Affiliations

2025–...	Metabolomics Society: Member
2025–...	Benelux Metabolomics Center: Member
2022–...	Human Proteome Organization – Proteomics Standards Initiative: Chair of the Quality Control Working Group
2021–...	Human Proteome Organization: Member
2017–...	European Bioinformatics Community for Mass Spectrometry: Member
2016–2022	Human Proteome Organization – Proteomics Standards Initiative: Secretary of the Quality Control Working Group
2014–...	International Society for Computational Biology: Member
2013–...	Belgian Proteomics Association: Member
2013–...	American Society for Mass Spectrometry: Member